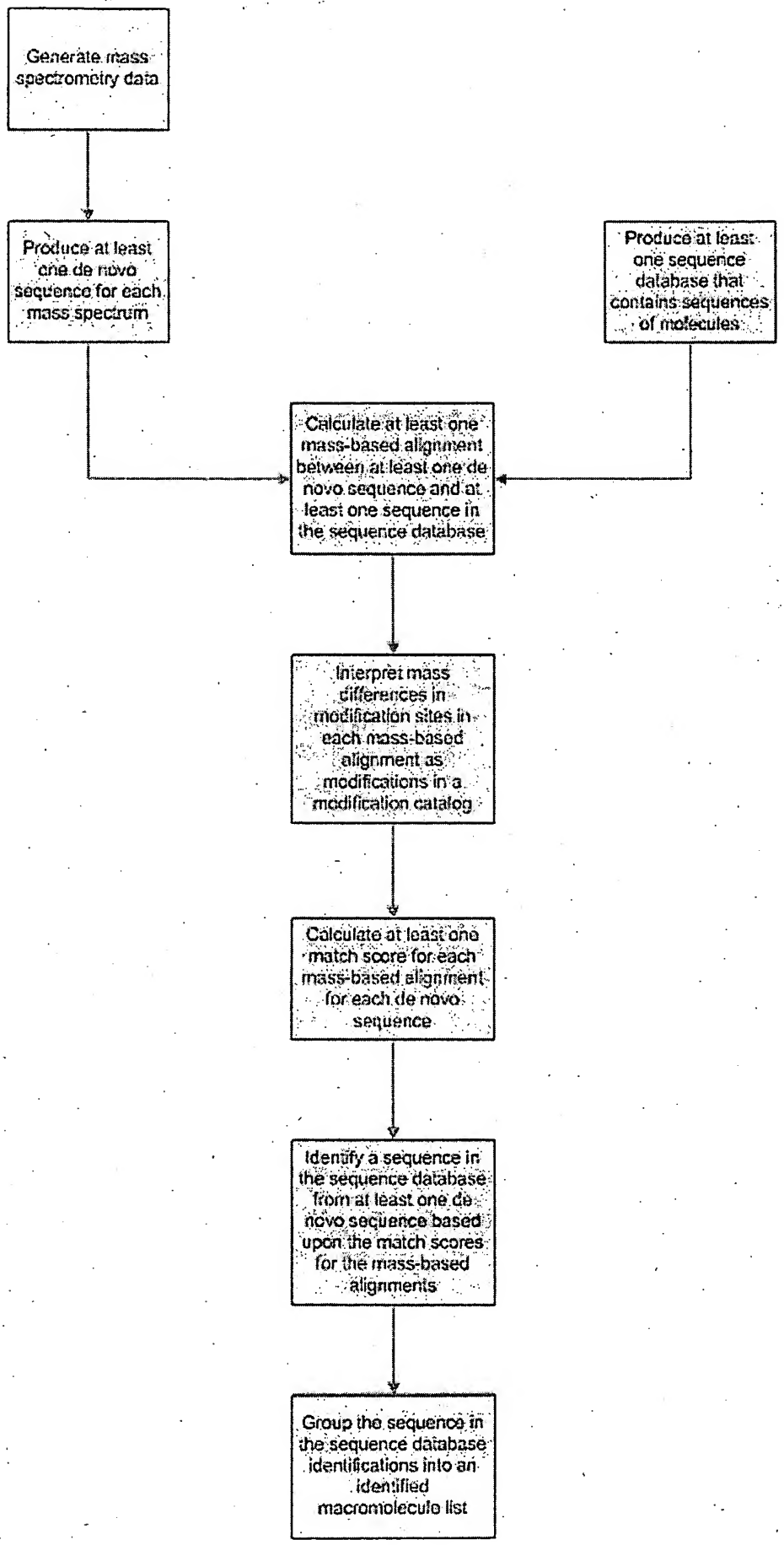

Generate mass spectrometry data
Produce at least one de novo sequence for each mass spectrum
Produce at least one sequence database that contains sequences of molecules
Calculate at least one mass-based alignment between at least one de novo sequence and at least one sequence in the sequence database
Interpret mass differences in modification sites in each mass-based alignment as modifications in a modification catalog
Calculate at least one match score for each mass-based alignment for each de novo sequence
Identify a sequence in the sequence database from at least one de novo sequence based upon the match scores for the mass-based alignments
Group the sequence in the sequence database identifications into an identified macromolecule list

FIG. 1

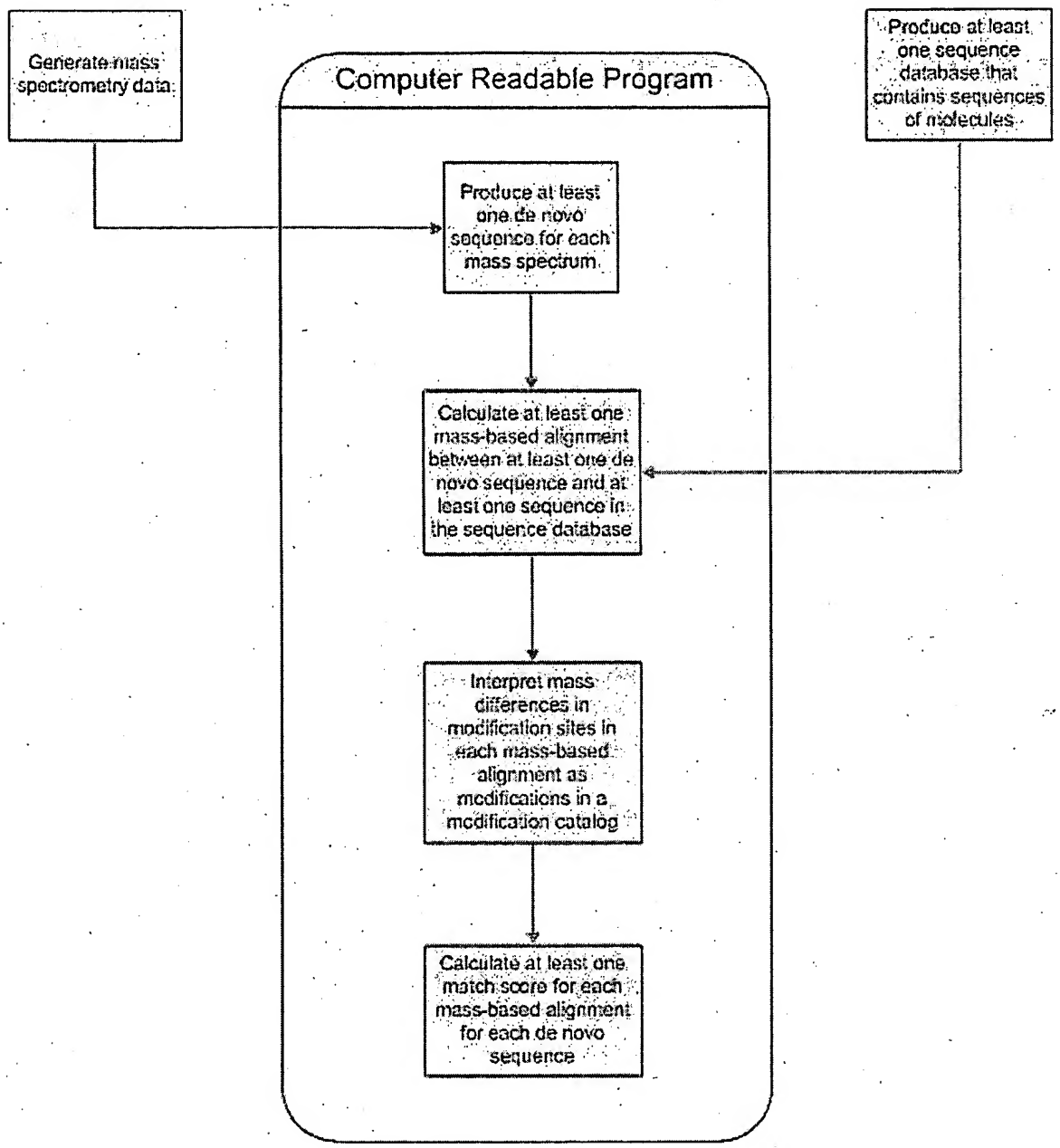

Generate mass spectrometry data
Computer Readable Program
Produce at least one sequence database that contains sequences of molecules
Produce at least one de novo sequence for each mass spectrum
Calculate at least one mass-based alignment between at least one de novo sequence and at least one sequence in the sequence database
Interpret mass differences in modification sites in each mass-based alignment as modifications in a modification catalog
Calculate at least one match score for each mass-based alignment for each de novo sequence

FIG. 2

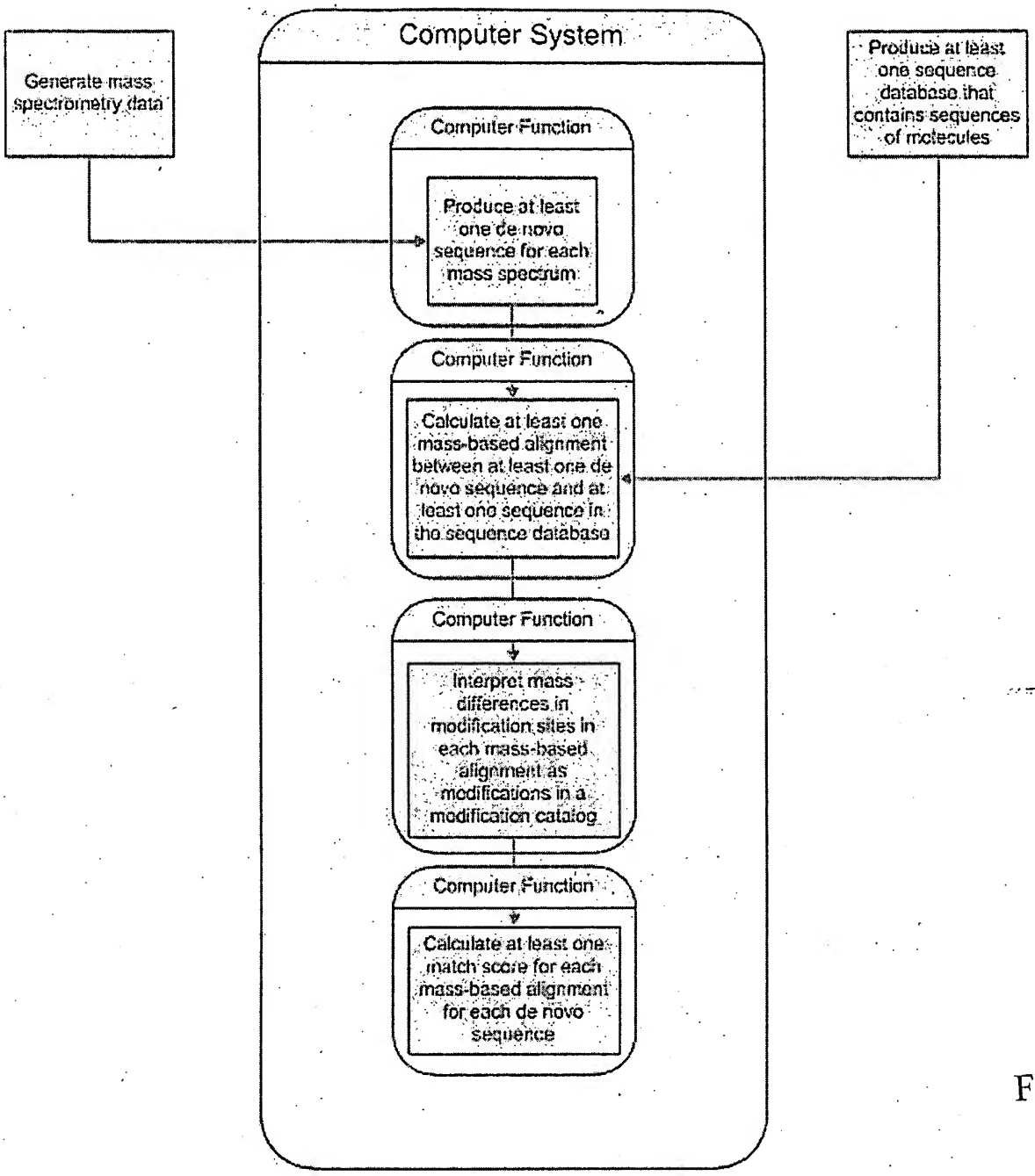

Computer System
Generate mass spectrometry data
Produce at least one sequence database that contains sequences of molecules
Computer Function
Produce at least one de novo sequence for each mass spectrum
Computer Function
Calculate at least one mass-based alignment between at least one de novo sequence and at least one sequence in the sequence database
Computer Function
Interpret mass differences in modification sites in each mass-based alignment as modifications in a modification catalog
Computer Function
Calculate at least one match score for each mass-based alignment for each de novo sequence

FIG. 3

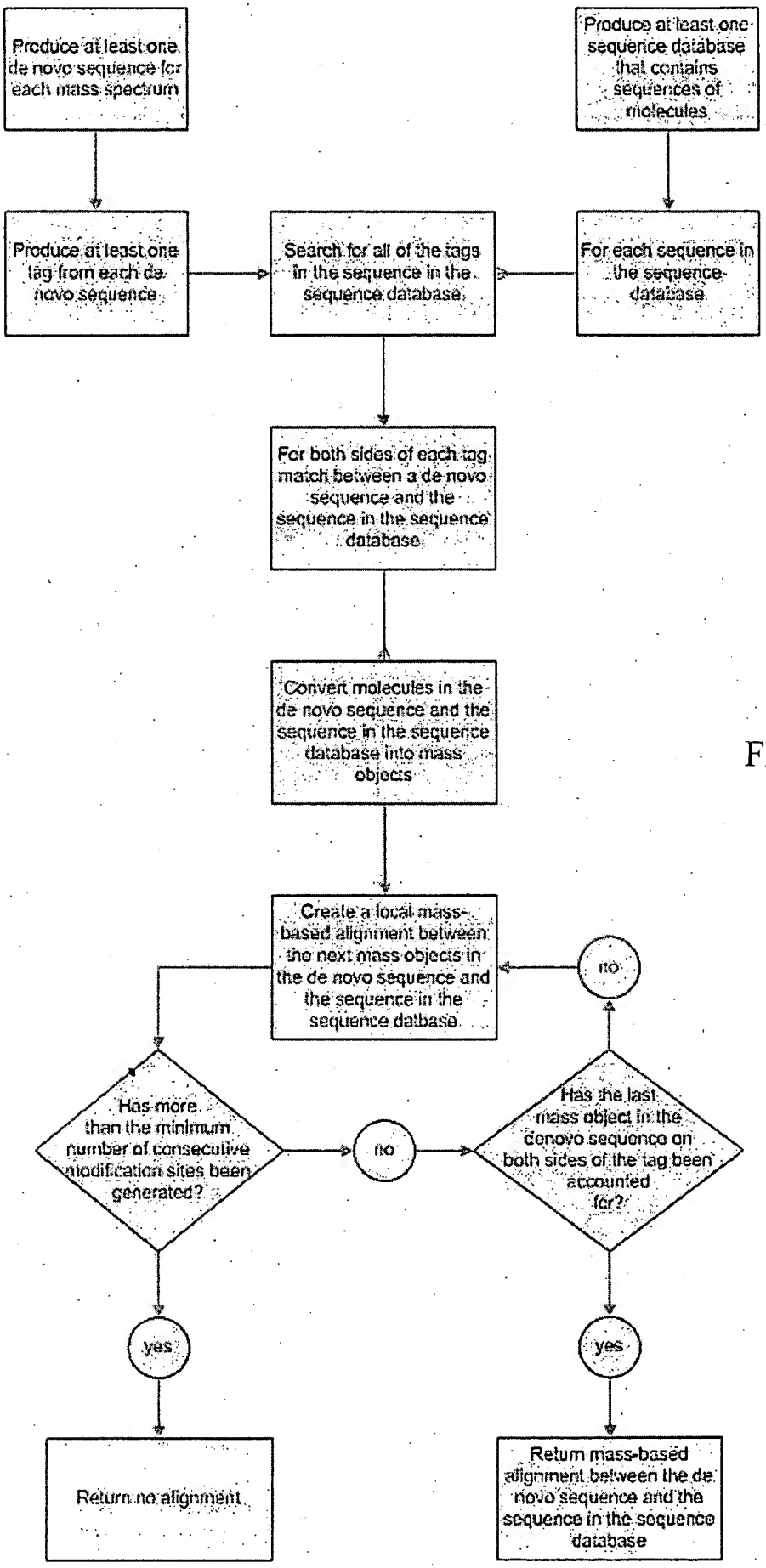

Produce at least one de novo sequence for each mass spectrum
Produce at least one sequence database that contains sequences of molecules
Produce at least one tag from each de novo sequence
Search for all of the tags in the sequence in the sequence database
For each sequence in the sequence database
For both sides of each tag match between a de novo sequence and the sequence in the sequence database
Convert molecules in the de novo sequence and the sequence in the sequence database into mass objects
Create a local mass-based alignment between the next mass objects in the de novo sequence and the sequence in the sequence database
no
Has more than the minimum number of consecutive modification sites been generated?
no
Has the last mass object in the denovo sequence on both sides of the tag been accounted for?
yes
yes
Return no alignment
Return mass-based alignment between the de novo sequence and the sequence in the sequence database

FIG. 4

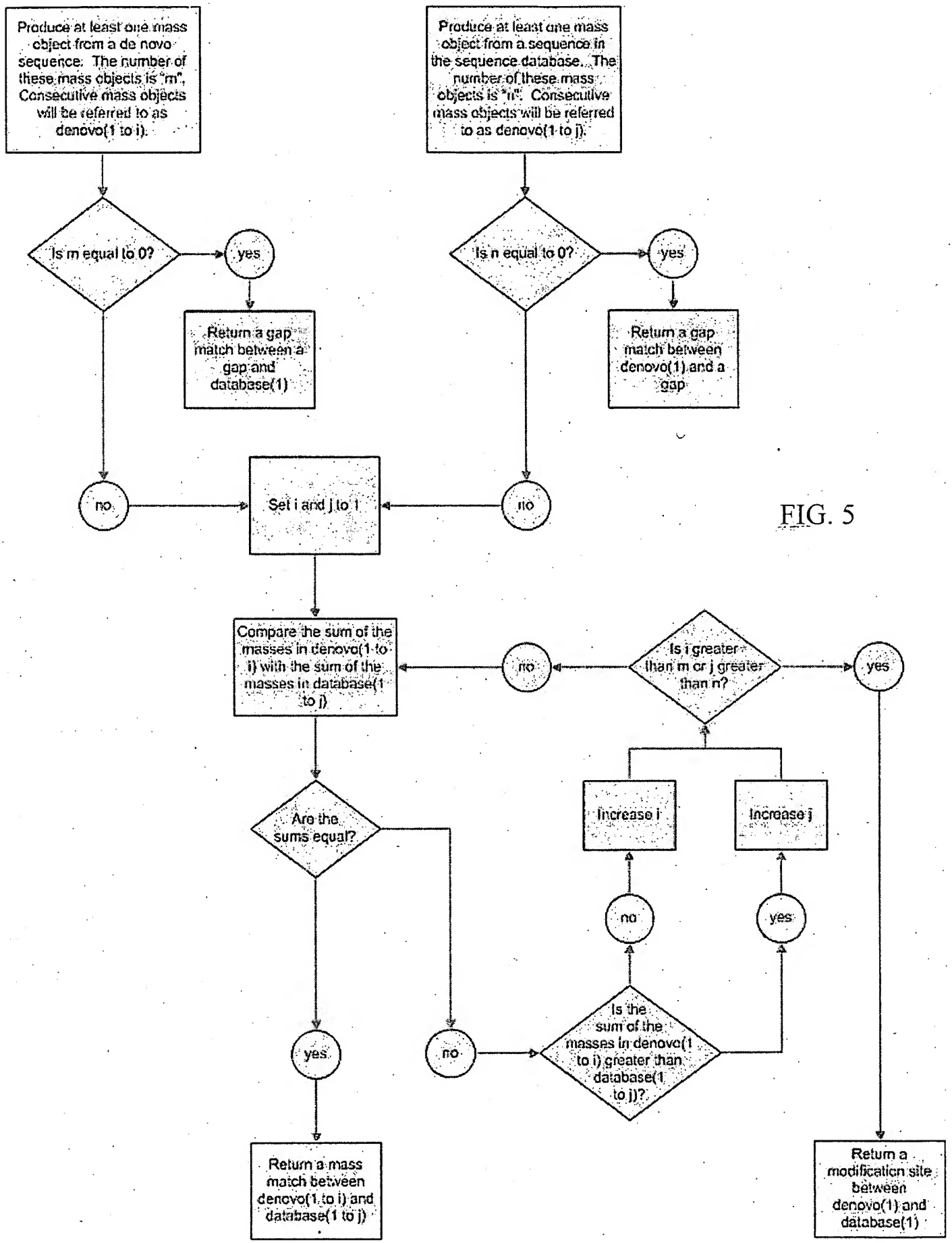

Produce at least one mass object from a de novo sequence. The number of these mass objects is "m". Consecutive mass objects will be referred to as denovo(1 to i).
Produce at least one mass object from a sequence in the sequence database. The number of these mass objects is "n". Consecutive mass objects will be referred to as denovo(1 to j).
Is m equal to 0?
yes
Return a gap match between a gap and database(1)
Is n equal to 0?
yes
Return a gap match between denovo(1) and a gap
no
Set i and j to 1
no
Compare the sum of the masses in denovo(1 to i) with the sum of the masses in database(1 to j)
no
Is i greater than m or j greater than n?
yes
Are the sums equal?
Increase i
Increase j
no
yes
yes
no
Is the sum of the masses in denovo(1 to i) greater than database(1 to j)?
Return a mass match between denovo(1 to i) and database(1 to j)
Return a modification site between denovo(1) and database(1)

FIG. 5

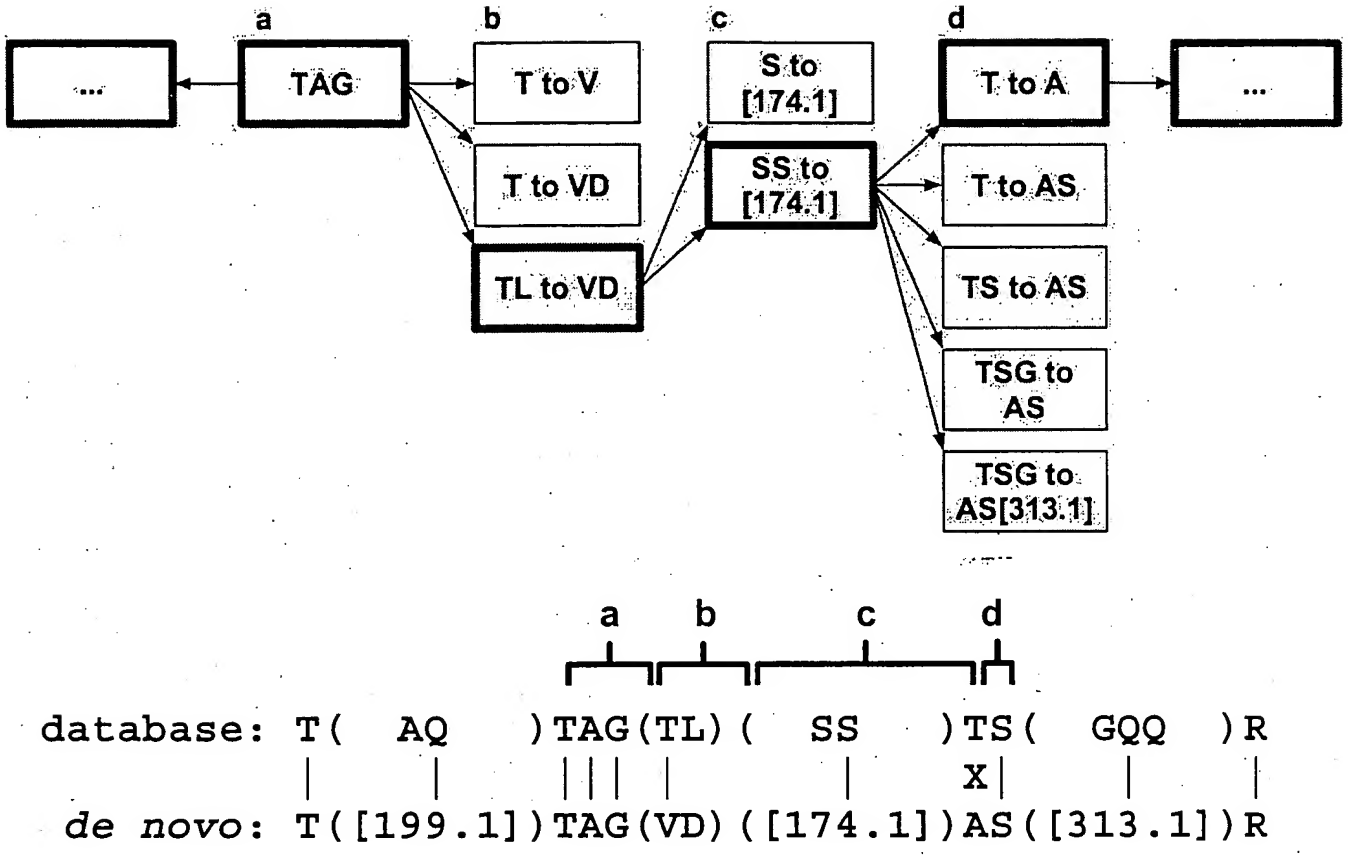
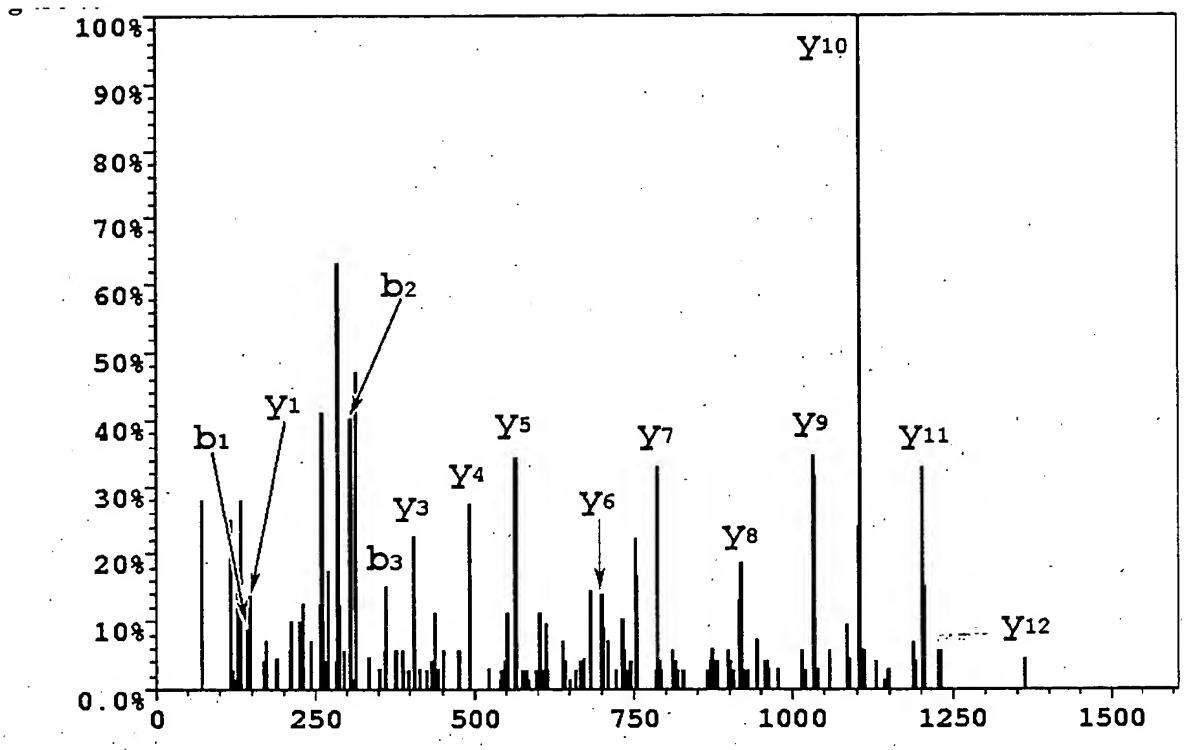

a
b
c
d
...
TAG
T to V
T to VD
TL to VD
S to [174.1]
SS to [174.1]
T to A
T to AS
TS to AS
TSG to AS
TSG to AS[313.1]
...
a
b
c
d
database: T(AQ)TAG(TL)(SS)TS(GQQ)R
de novo: T([199.1])TAG(VD)([174.1])AS([313.1])R

FIG. 6



***De Novo* Sequence:**

[144.1]SATADESHAGM[158.1]K

ALIGNMENT PROVIDED BY ONE EMBODIMENT OF THE PRESENT INVENTION

ALBU_BOVIN Serum Albumin Precursor

a FAK(T)(CcV)ADESHAG(CcE)KSLH

X

b ([144.1])(SAT)ADESHAG(M[158.1])K

c d

FIG. 7

FIG. 8(a)

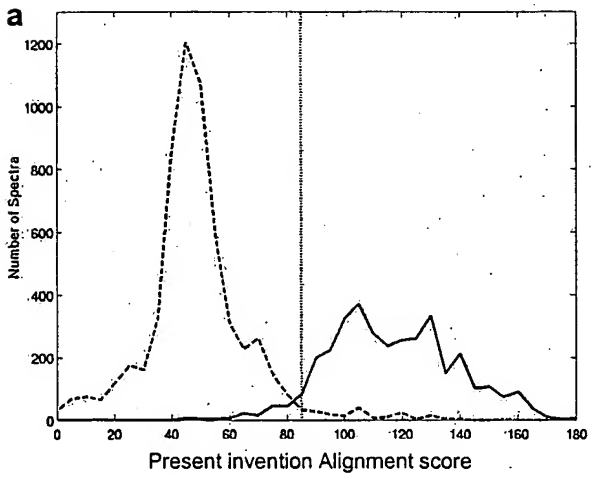


FIG. 8(b)

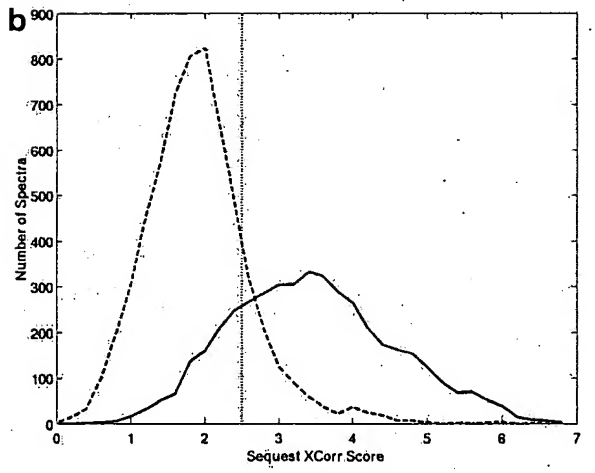
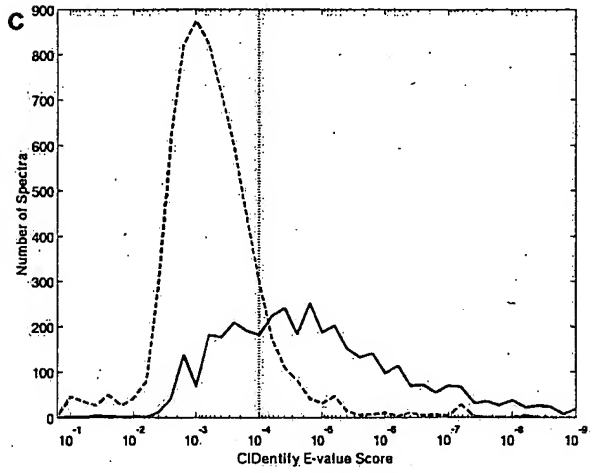


FIG. 8(c)



PEAKS PROVIDED IN ONE EMBODIMENT OF THE PRESENT INVENTION

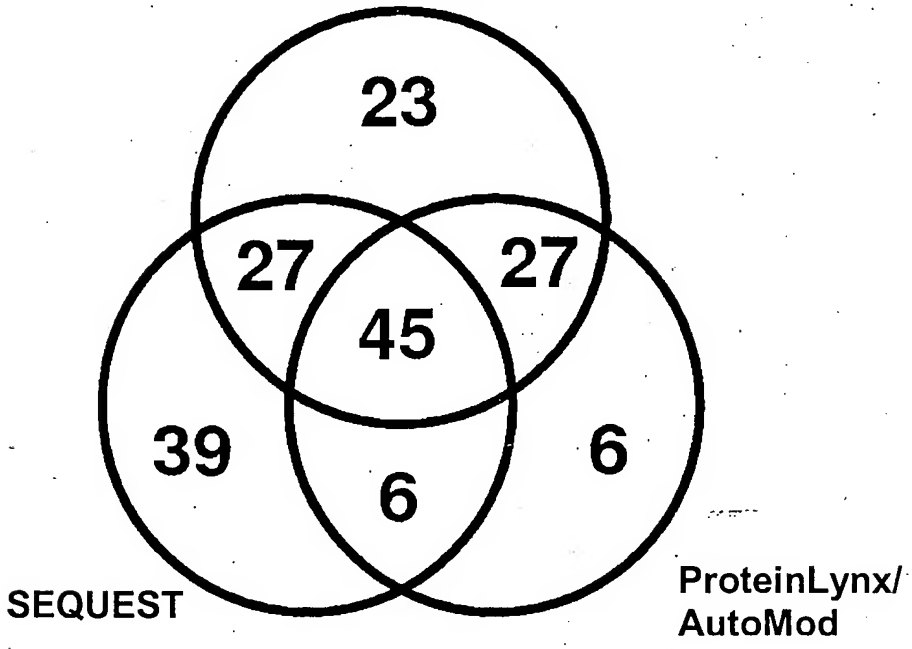
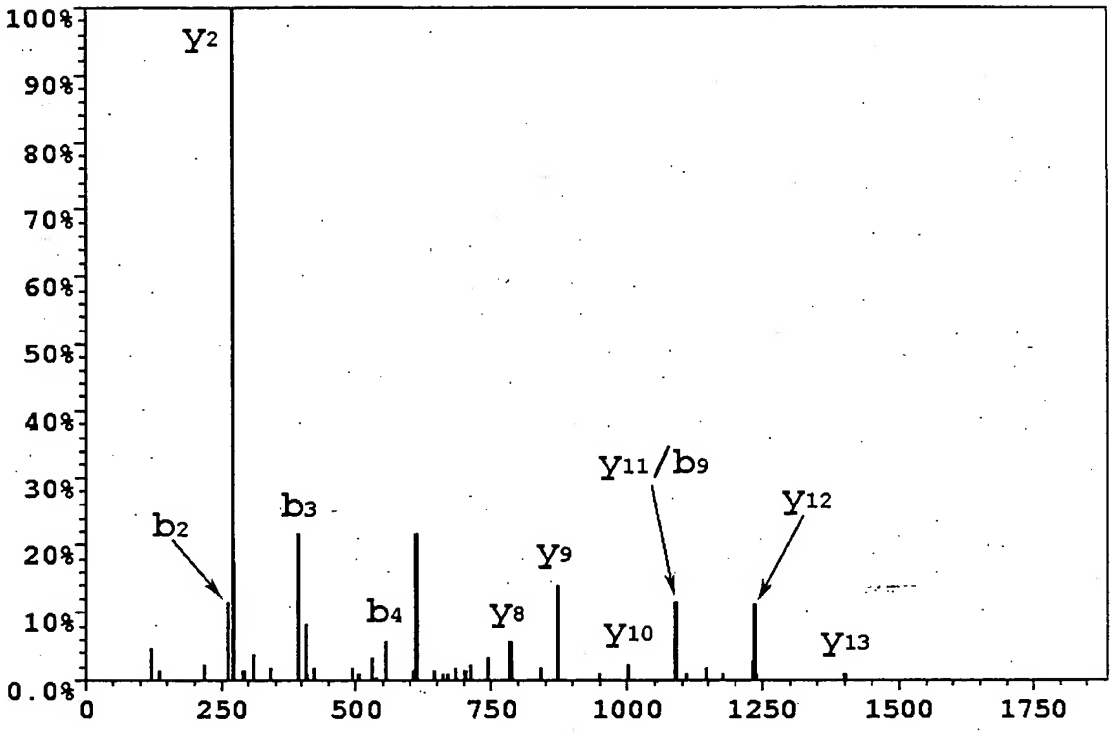


FIG. 9



***De Novo* Sequence:**

[554.2]FS[128.1]SSSG[283.1]PR

ALIGNMENT PROVIDED BY ONE EMBODIMENT OF THE PRESENT INVENTION

```
TRFL_HUMAN Lactotransferrin Precursor
SCK( FDEY  )FS(   Q   )SC(  APGSD  )PRSNL
      |    ||    |     |X     |      ||
  ([554.2])FS([128.1])SS(SG[283.1])PR
                          ⌊
                          a
```

FIG. 10